

2-Thiopheneacetic acid, methyl ester

Other names:	Methyl 2-thiopheneacetate Methyl thiophene-2-acetate methyl thiophen-2-acetate
Inchi:	InChI=1S/C7H8O2S/c1-9-7(8)5-6-3-2-4-10-6/h2-4H,5H2,1H3
InchiKey:	KNKIXYMOHMYZJR-UHFFFAOYSA-N
Formula:	C7H8O2S
SMILES:	COC(=O)Cc1cccs1
Mol. weight [g/mol]:	156.21

Physical Properties

Property code	Value	Unit	Source
cpl	249.80	J/mol×K	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
hvap	61.90 ± 1.40	kJ/mol	NIST Webbook
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-1.54		Cheméo Relay (1.0)
logp	1.464		Crippen Method
mcvol	113.820	ml/mol	McGowan Method
tb	482.86	K	Cheméo Relay (1.0)

Sources

Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives.

NIST Webbook:

McGowan Method:

Crippen Method:

Crippen Method:

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

<https://www.doi.org/10.1016/j.tca.2005.11.024>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C19432689&Units=SI>

<http://link.springer.com/article/10.1007/BF02311772>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpl:	Liquid phase heat capacity
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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